MS 2: Mass Spectrometry Methods

Time: Monday 16:30–18:15 Location: MS-H9

Invited Talk MS 2.1 Mon 16:30 MS-H9

Ion Laser InterAction Mass Spectrometry with fluoride molecular anions — •Martin Martschini[1], Karin Hain[1], Maki Honda[1,3], Johannes Lachner[2], Oscar Marchhart[1], Silke Merchel[1], Carlos Vivo-Vilches[2], and Robin Golser[1] — [1]University of Vienna, Faculty of Physics, Austria — [2]HZDR, Dresden, Germany — [3]NSRC, JAEA, Japan

AMS generally has the best abundance sensitivity for long-lived radionuclides, but the detection of ^{41}Ca, ^{90}Sr, ^{99}Tc, ^{135}Cs and ^{182}Hf in the general environment has been limited or even hampered by strong isobaric interferences. Using molecular fluoride anions, the novel technique of Ion Laser-InterAction Mass Spectrometry (ILIAMS) provides unprecedented isobar suppression for these nuclides of 10^4-10^8 inside an RFQ ion guide. Therein, isobaric molecules are efficiently eliminated via laser photodetachment. In addition, molecular interactions with the buffer gas further enhance isobar suppression, e.g. via breakup of KF_3^- into $KF_2^- + F$ or via O-pickup of WF_5^-. Thereby, the VERA-facility has recently achieved the most sensitive detection of ^{182}Hf and ^{90}Sr, the latter at the 15 attogram level. For ^{41}Ca, the blank level with CaF_3^- and ILIAMS is $^{41}Ca/^{40}Ca = (1.5^{+1.7}_{-1.5})\times10^{-15}$. Recent tests also demonstrated that ^{41}Ca can now be measured directly in stony meteorites with sample sizes down to 1-2 mg without performing any chemical preparation, i.e. in the presence of ∼1000 ppm K. This talk will review these benefits of fluoride anions with ILIAMS but also discuss the challenges involved like the strong parasitic ion current and the influence of excited molecules coming from a sputter ion source.

MS 2.2 Mon 17:00 MS-H9

A digital RF ion filter and trap combination for the MS SPIDOC prototype — •Florian Simke, Paul Fischer, and Lutz Schweikhard — Universität Greifswald, Institut für Physik, Felix-Hausdorff-Str. 6, 17489 Greifswald

The MS SPIDOC (Mass Spectrometry for Single Particle Imaging of Dipole Oriented protein Complexes) prototype [1] will deliver mass- and conformation separated samples of protein-based biomolecules for single-particle imaging analysis at the European X-Ray Free-Electron Laser Facility (XFEL)[2]. The design, simulation, and construction of one of its key modules is presented along with first offline results. The module consists of a linear-quadrupole filter assembly and a linear-quadrupole ion trap, both operated with digital radio frequencies. The restriction to keep investigated biomolecules as native as possible leads to a design that separates ion filtering and accumulation/trapping. The module is able to filter ions of interest with mass-to-charge ratios of up to $m/z \approx 12000$ Th. The ion trap is utilized to collect and bunch incoming ions from a continuous source and eject them with a narrow temporal width for downstream analysis and X-ray interaction.

[1] C. Uetrecht et al., Native mass spectrometry provides sufficient ion flux for XFEL single-particle imaging, Journal of Synchrotron Radiation 26 (3) (2019) 653-659. doi:10.1107/S1600577519002686
[2] Europe turns on bright x-ray source, Nature Photon; 11 (2017) 609-609, doi:https://doi.org/10.1038/s41566-017-0025-z

MS 2.3 Mon 17:15 MS-H9

Production and characterization of standard particles for rL-SNMS calibration — Stefan Bister, •Paul Hanemann, Manuel Raiwa, Sandra Reinhard, Darcy van Eerten, and Clemens Walther — Institute of Radioecology and Radiation Protection, Leibniz University Hannover

Resonant laser secondary neutral mass spectrometry (rL-SNMS) is a non-destructive method that combines high sensitivity and resolution of ToF-SIMS with high element selectivity of resonant laser ionisation. One main application is the determination of isotope ratios on individual micro particles of spent nuclear fuel from the Chernobyl exclusion zone (CEZ). Standard materials are needed for dealing with isobaric interferences such as 238U and 238Pu as well as differences in the laser ionisation and sputter efficiencies for different elements and isotopes. This work produced particles via Fe-coprecipitation to achieve homogeneous U and Pu bearing particles. Isotopes with different mass numbers were used to determine relative ionisation efficiencies without isobaric interferences. The homogeneity of U and Pu in the particles was confirmed by ToF-SIMS and EDX measurements. On several particles Pu-resonant measurement were performed to investigate the suppression of non-resonant U. It was shown that the suppression is high enough to be able to detect 238Pu in a particle with a 1E5 higher 238U content, as found in "hot particles" from the CEZ. RL-SNMS measurements of produced particles containing only different U isotopes allowed the investigation of isotope effects in the resonant laser ionisation.

MS 2.4 Mon 17:30 MS-H9

Dissociative electron attachment studies with nitro-heterocyclic aromatic compounds — •Muhammad Saqib, Eugene Arthur-Baidoo, Milan Ončák, and Stephan Denifl — Institute of Ion Physics and Applied Physics, University of Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria

Nitro-heterocyclic aromatic compounds have a wide range of applications in medicine. Due to their specific toxicity, which is defined by their reduction to the biologically active form in the lack of oxygen, these compounds play a crucial role in targeting the hypoxic tumor cell during cancer treatment. We have studied the formation of anions following electron attachment to nitro-heterocyclic compounds in the gas phase. By using a crossed electron/molecular beams experiments with mass spectrometric detection of the anions, we studied electron attachment to 2-nitrofuran, 3-nitro-1,2,4-triazole, and 1H-1,2,4-triazole molecules. Dissociative electron attachment and non-dissociative electron attachment were observed. The obtained results of electron attachment to 2-nitrofuran indicate that low-energy electrons, with kinetic energies from 0 eV to 12 eV, effectively decompose the molecule and lead to a large variety of charged fragments and radicals with the nitrogen dioxide anion as the most abundant fragment anion. The experimental study was supported by thermochemical threshold calculations. This work was supported by the FWF, Vienna (P30332).

MS 2.5 Mon 17:45 MS-H9

Investigation of mass-scale drift effects in the milli-mass range using MC-ICP-MS — •Axel Pramann, Janine Noordmann, and Olaf Rienitz — Physikalisch-Technische Bundesanstalt; Braunschweig, Germany

During the application of an MC-ICP magnetic sector field mass spectrometer, severe mass drift effects in the milli-mass range in the high resolution mode (M/ΔM = 8000) have been observed [1]. Their potential origins, experimental prevention, and the consequences are outlined. Additional simulations were performed using silicon enriched in 28Si as the main element in this investigation. One background is the fact that a drift of the mass scale influences the determination of isotope ratios strongly. For example, the signal-plateau width of 29Si+ in Si highly enriched in 28Si exhibits an extremely narrow mass plateau width of ΔM = 4 * 10-3 u, one of the smallest plateaus routinely investigated in isotope ratio measurements. A change of the magnetic field B, the acceleration voltage Uacc or the ESA voltage UESA by 0.01% induces respective changes of the mass scale of 6 * 10-3 u, 3 * 10-3 u, and 1 * 10-3 u, respectively. Electrical charging/discharging effects in the MS were observed and suggested to be affecting the mass scale stability. Therefore, the instrument was completely dismantled, grounded, and carefully reinstalled. Subsequent stability tests yielded a negligible mass drift of ΔM/Δt = 0.001 u/8 h, allowing for the measurement of isotope ratios with lowest uncertainty.

[1] A. Pramann, J. Noordmann, O. Rienitz, J. Mass Spectrom. 56:e4732 (2021)

MS 2.6 Mon 18:00 MS-H9

The PUMA offline ion source for high-intensity, purified ion bunches — •Clara Klink, Alexandre Obertelli, Frank Wienholtz, and Moritz Schlaich — TU Darmstadt, IKP, Darmstadt, Deutschland

The antiProton Unstable Matter Annihilation (PUMA) experiment aims at investigating the nucleonic composition in the tail of the nuclear density distribution of stable and exotic nuclei using antiprotons. The combined charge of the reaction products, which originate from the annihilation of the antiproton with the nucleons on the nucleus' surface, will allow for a determination of neutron and proton densities. Inter alia, PUMA plans on performing experiments with low-energy antiprotons from the ELENA facility of CERN with a broad range of

stable isotopes from an offline ion source to observe their behaviour during antiprotonic annihilation. The beamline, which transports the stable ions to the experimental site of PUMA, must meet several requirements to reliably forward the beam and shape it according to our needs. The ions are mass-separated with a multi-reflection time-of-flight mass spectrometer and then accumulated, bunched and cooled with a buffer gas in a linear Paul trap. Strict vacuum requirements due to the attached antiproton beamline (p < 10e-11 mbar) must be considered. This talk will give an introduction to the setup and operation of the offline ion source beamline, which will be essential for achieving the first physics results of PUMA.